A scaling hypothesis for PEPS

Laurens Vanderstraeten
University of Ghent

Overview

Introduction: PEPS for 2-D quantum systems and 3-D stat-mech

Variational optimization of PEPS fixed points

PEPS for critical systems: a scaling hypothesis

Outlook

Bram Vanhecke, Juraj Hasik, Frank Verstraete, LV
arXiv:2102.03143

Overview

Introduction: PEPS for 2-D quantum systems and 3-D stat-mech

Variational optimization of PEPS fixed points

PEPS for critical systems: a scaling hypothesis

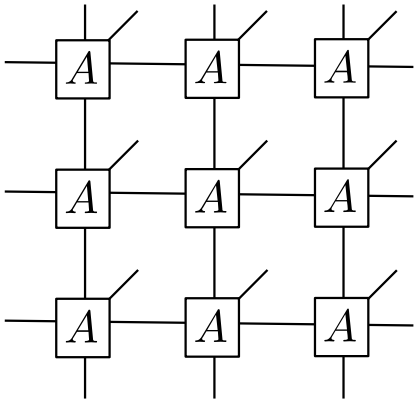
Outlook

Bram Vanhecke, Juraj Hasik, Frank Verstraete, LV
arXiv:2102.03143

Introduction

Projected entangled-pair states (PEPS) are variational wavefunctions for 2-D lattice systems

$$|\Psi(A)\rangle_{\mathrm{PEPS}} =$$



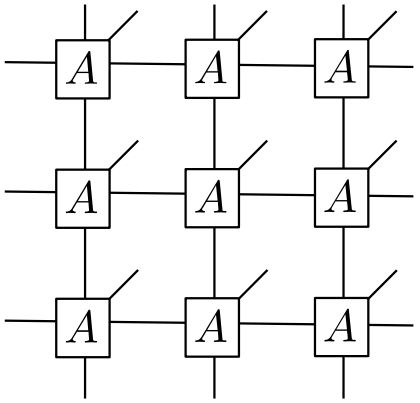
→ formulated directly in the thermodynamic limit

→ parametrized by a single local tensor
(larger unit cells possible)

Introduction

Projected entangled-pair states (PEPS) are variational wavefunctions for 2-D lattice systems

$$|\Psi(A)\rangle_{\mathrm{PEPS}} =$$



→ formulated directly in the thermodynamic limit

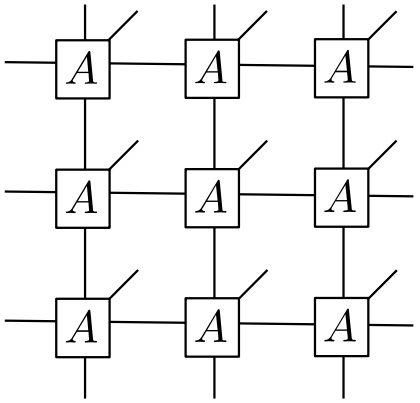
→ parametrized by a single local tensor
(larger unit cells possible)

→ ground-state wavefunctions for 2-D quantum lattice systems
(spins, bosons, electrons)

Introduction

Projected entangled-pair states (PEPS) are variational wavefunctions for 2-D lattice systems

$$|\Psi(A)\rangle_{\mathrm{PEPS}} =$$



→ formulated directly in the thermodynamic limit

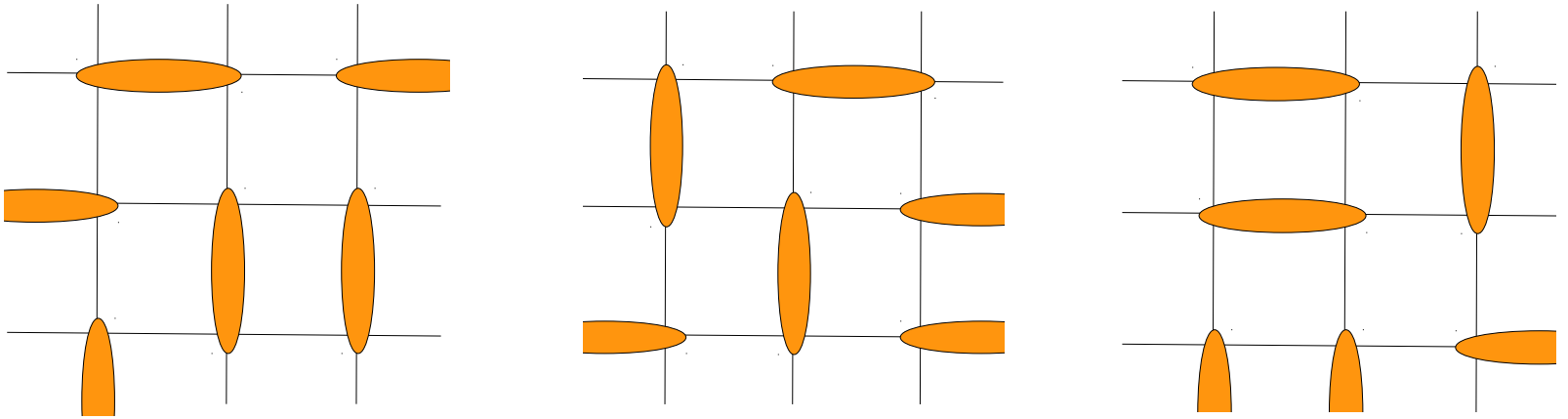
→ parametrized by a single local tensor
(larger unit cells possible)

→ ground-state wavefunctions for 2-D quantum lattice systems
(spins, bosons, electrons)

→ transfer-matrix fixed points for 3-D stat-mech systems

Introduction

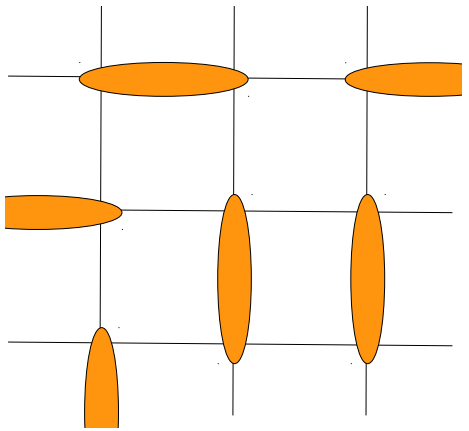
Example: dimer-covering problem

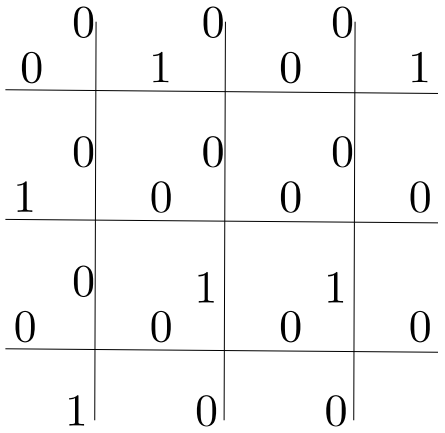


→ how does the number of dimer coverings scale with system size?

Introduction

Example: dimer-covering problem

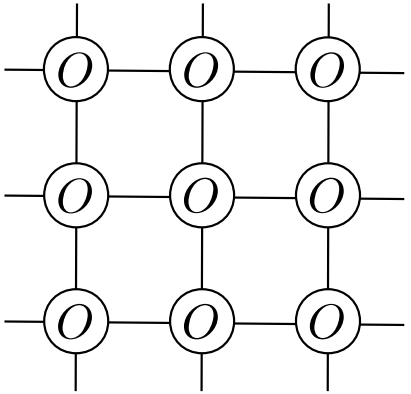


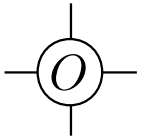


dimer rule on
the vertices

Tensor network that sums all allowed configurations

$$\mathcal{Z}_{\mathrm{dimer,2d}} =$$



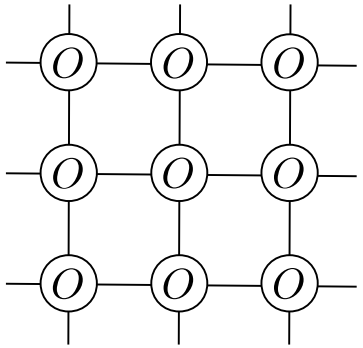
with  $= \begin{cases} 1, & \text{one index has value 1} \\ 0, & \text{otherwise} \end{cases}$

→ how does this number scale with system size?

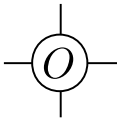
Introduction

Example: dimer-covering problem

$$\mathcal{Z}_{\mathrm{dimer,2d}} =$$



with



$$= \begin{cases} 1, & \text{one index has value 1} \\ 0, & \text{otherwise} \end{cases}$$

Contraction of infinite network gives extremely precise results
(this is a critical model)

exact $S = 0.2915609040$

Baxter's CTMRG (D=6, IBM-360) $S = 0.29146021876$

boundary MPS (D=250, laptop) $S = 0.2915608913$

→ variational results!

TABLE I. The values of κ/s obtained from the $r = 1, 2, \cdots, 6$ approximations for $s = 1.0$, 4.0, 10.0, and ∞, together with the values obtained by geometric extrapolation from the 4, 5, 6 results.

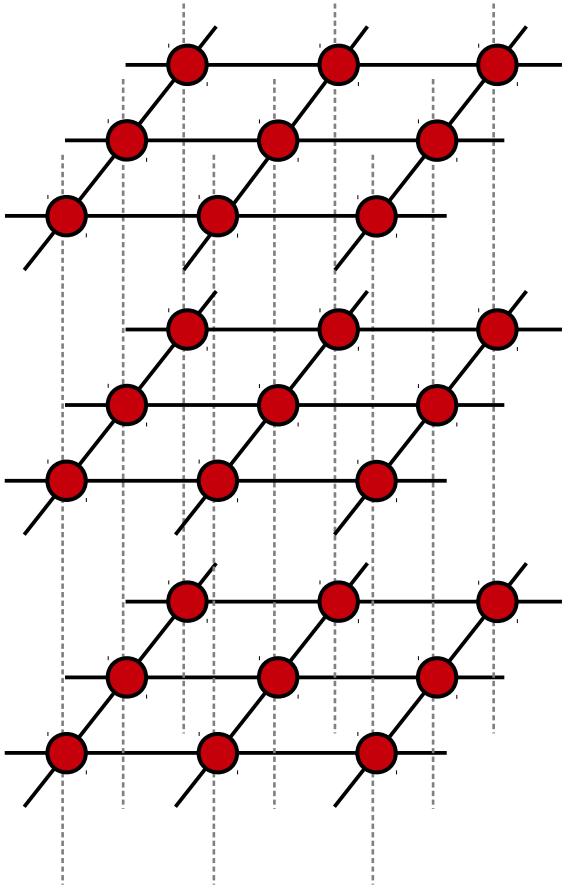
r	κ/s			
	$s = 1.0$	$s = 4.0$	$s = 10.0$	$s = \infty$
1	1.937416664	1.444670083	1.356095932	1.299038106
2	1.940215341	1.460590906	1.381143005	1.335033348
3	1.940215344	1.460623453	1.381458447	1.337338271
4	1.940215351	1.460629381	1.381506501	1.337984697
5	1.940215351	1.460629397	1.381508315	1.338250017
6	1.940215351	1.460629398	1.381508512	1.338380390
Extrap-olated	1.940215351	1.460629398	1.381508536	1.338506344

Baxter 1968

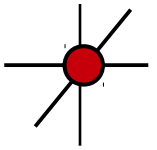
Introduction

Example: dimer-covering problem

$$\mathcal{Z}_{\mathrm{dimer,3d}} =$$



with the tensor



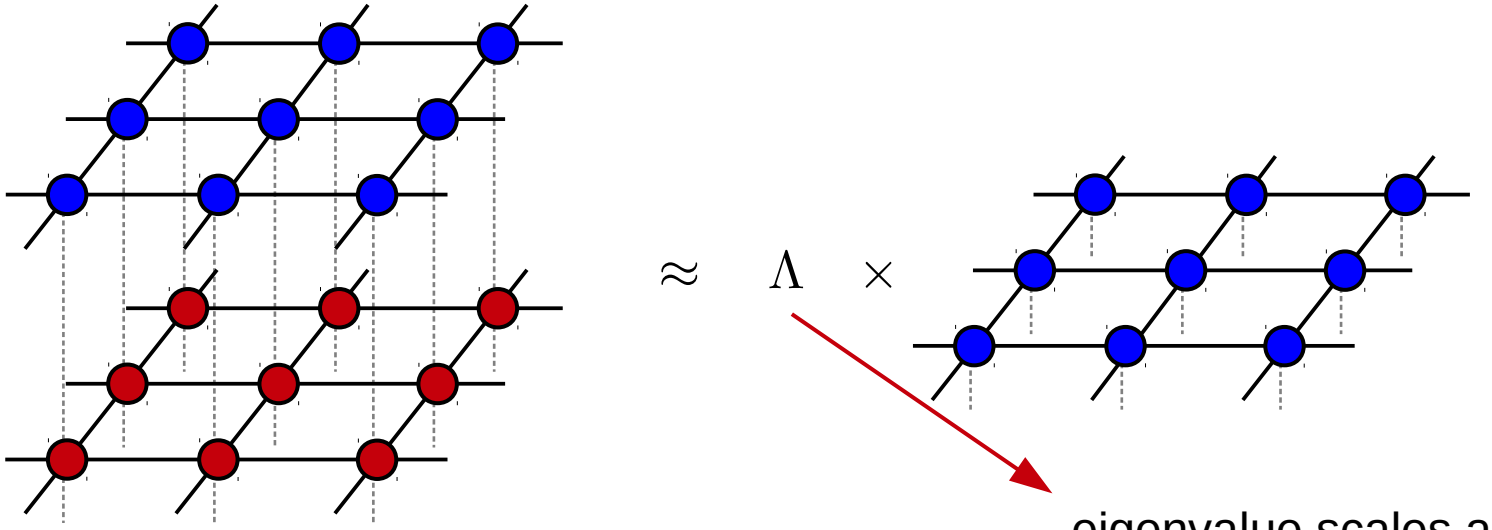
$$= \begin{cases} 1, & \text{one index has value 2} \\ 0, & \text{otherwise} \end{cases}$$

→ plane-to-plane transfer matrix

Introduction

Example: dimer-covering problem

→ approximate the fixed point of the transfer matrix as a PEPS



eigenvalue scales as

$$\Lambda = \lambda^{N_x N_y}$$

such that entropy density is given by

$$S = \log \lambda$$

→ how do we optimize PEPS fixed points, and how do extrapolate data?

Overview

Introduction: PEPS for 2-D quantum systems and 3-D stat-mech

Variational optimization of PEPS fixed points

PEPS for critical systems: a scaling hypothesis

Outlook

Bram Vanhecke, Juraj Hasik, Frank Verstraete, LV
arXiv:2102.03143

Variational optimization

An optimal PEPS approximation is characterized by the variational principle

→ for quantum Hamiltonians

$$A = \arg\min_A \left(\frac{\langle \Psi(A) | \mathcal{H} | \Psi(A) \rangle}{\langle \Psi(A) | \Psi(A) \rangle} \right)$$

gradient-based methods were developed that optimize
the variational cost function directly

Corboz, PRB 94, 035133 (2016)
LV, Haegeman, Corboz, Verstraete, PRB 94, 155123 (2016)

→ for transfer matrices

$$A = \arg\min_A \left(-\log \frac{\langle \Psi(A) | \mathcal{T} | \Psi(A) \rangle}{\langle \Psi(A) | \Psi(A) \rangle} \right)$$

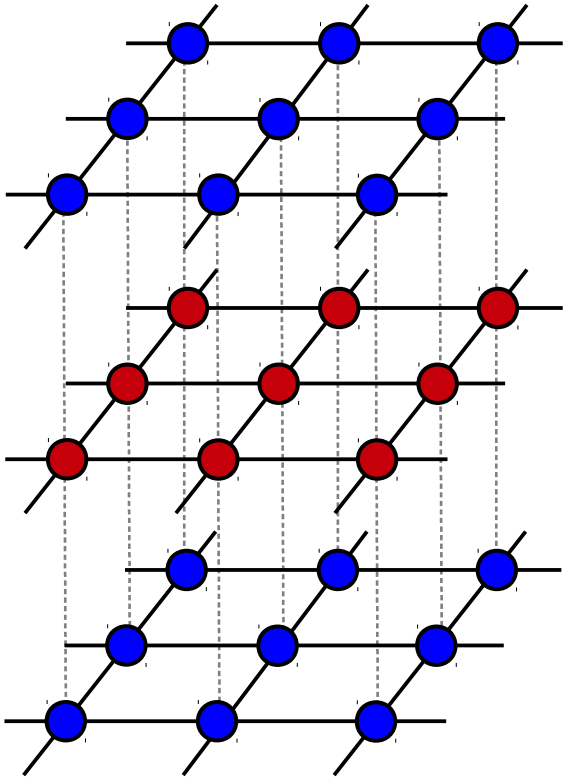
similar gradient-based method for optimization

Nishino et al, Nucl. Phys. B 575, 504 (2000)
LV, Vanhecke, Verstraete, PRE 98, 042145 (2018)

Variational optimization

Direct variational optimization of the free energy

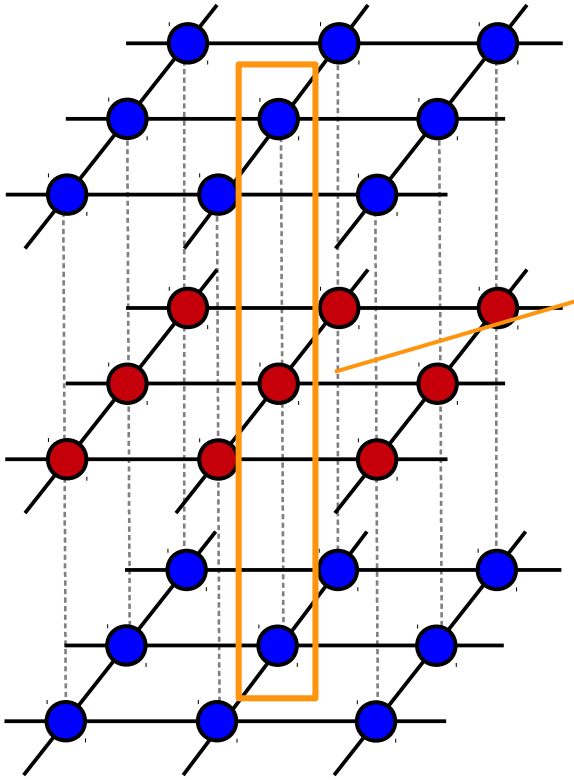
$$A = \arg\min_{A} \left(-\log \frac{\langle \Psi(A) | \mathcal{T} | \Psi(A) \rangle}{\langle \Psi(A) | \Psi(A) \rangle} \right)$$



Variational optimization

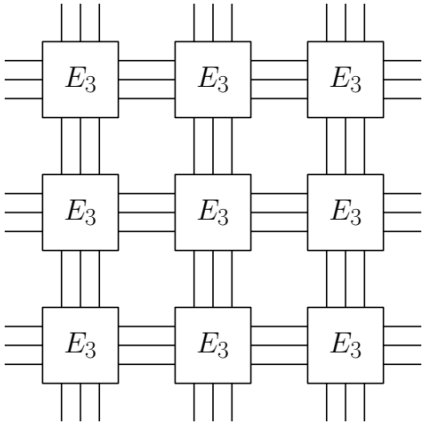
Direct variational optimization of the free energy

$$A = \arg\min_A \left(-\log \frac{\langle \Psi(A) | \mathcal{T} | \Psi(A) \rangle}{\langle \Psi(A) | \Psi(A) \rangle} \right)$$



top view

$\langle \Psi(A) | \mathcal{T} | \Psi(A) \rangle =$

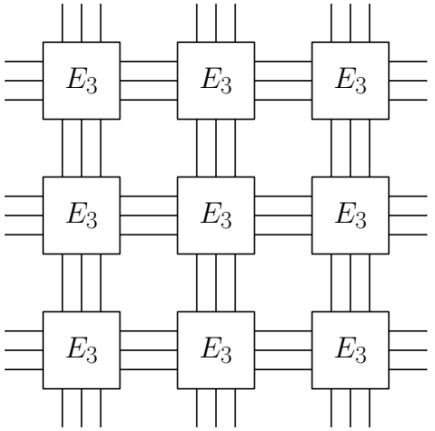


evaluation of the variational cost function requires the contraction of an infinite three-layer tensor network

Variational optimization

Evaluation of the variational cost function requires the contraction of an infinite three-layer tensor network

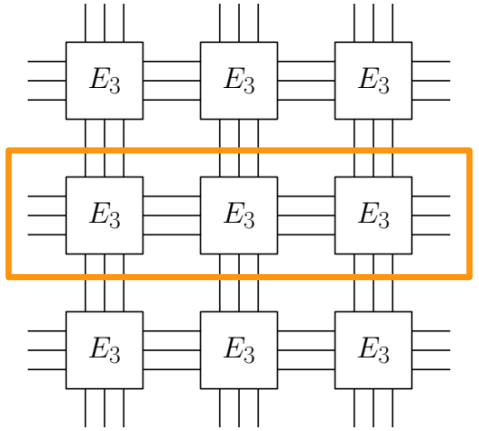
$$\langle \Psi(A) | \, \mathcal{T}_{2\mathrm{d}} \, | \Psi(A) \rangle =$$



Variational optimization

Evaluation of the variational cost function requires the contraction of an infinite three-layer tensor network

$$\langle \Psi(A) | \, \mathcal{T}_{2\mathrm{d}} \, | \Psi(A) \rangle =$$

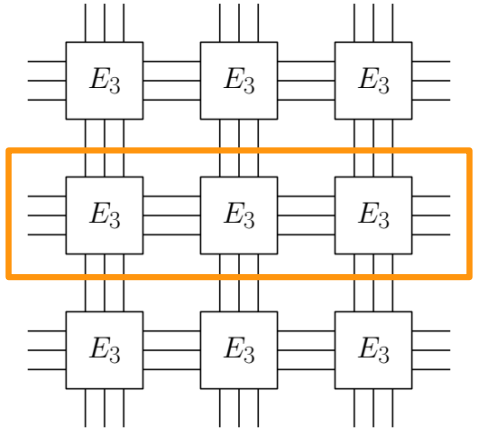


1-D transfer matrix

Variational optimization

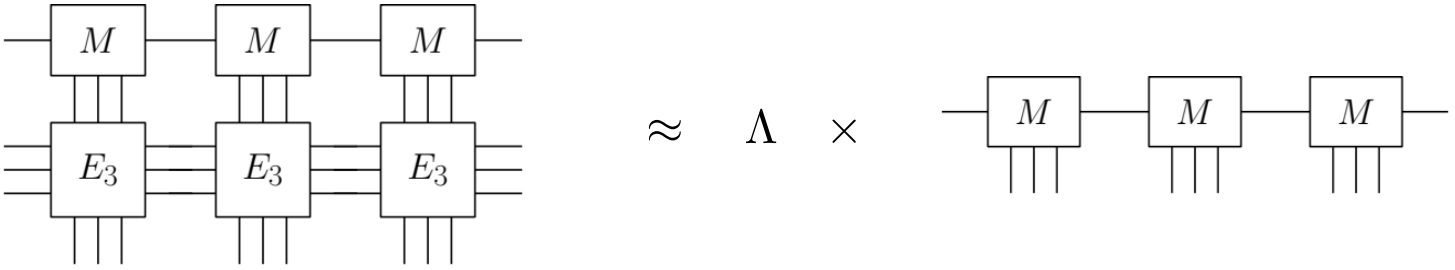
Evaluation of the variational cost function requires the contraction of an infinite three-layer tensor network

$$\langle \Psi(A)| \mathcal{T}_{2\mathrm{d}} |\Psi(A)\rangle =$$



→ 1-D transfer matrix

→ approximate the boundary of the 1-D transfer matrix as an MPS



→ apply the variational principle for the boundary contraction

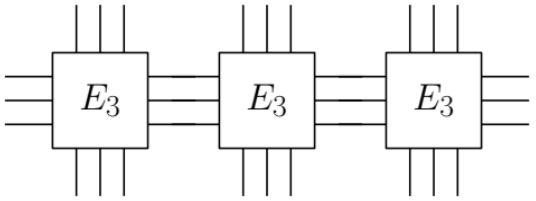
$$M = \arg\min_{M} \left(-\log \frac{\langle \Psi(M)| \mathcal{T}_{1\mathrm{d}} |\Psi(M)\rangle}{\langle \Psi(M)|\Psi(M)\rangle} \right)$$

Variational optimization

Apply the variational principle for the boundary contraction

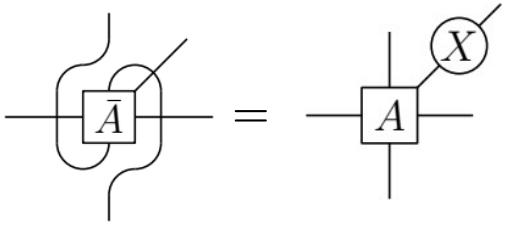
$$M = \arg\min_M \left(-\log \frac{\langle \Psi(M) | \, \mathcal{T}_{1\mathrm{d}} \, | \Psi(M) \rangle}{\langle \Psi(M) | \Psi(M) \rangle} \right)$$

with

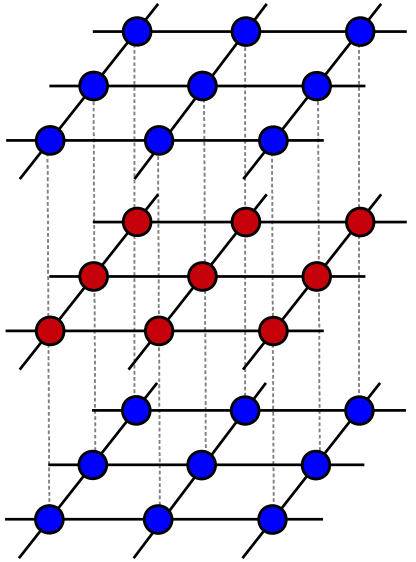
$\mathcal{T}_{1\mathrm{d}} =$ 

→ the transfer matrix has to be hermitian!

Impose symmetry constraints on the PEPS tensors



→ implies that transfer matrix is hermitian,
and we can use variational algorithms



Variational optimization

Hierarchy of variational principles

→ boundary PEPS $A = \arg\min_A \left(-\log \frac{\langle \Psi(A) | \mathcal{T}_{2\mathrm{d}} | \Psi(A) \rangle}{\langle \Psi(A) | \Psi(A) \rangle} \right)$

control parameter: PEPS bond dimension D

→ boundary MPS $M = \arg\min_M \left(-\log \frac{\langle \Psi(M) | \mathcal{T}_{1\mathrm{d}} | \Psi(M) \rangle}{\langle \Psi(M) | \Psi(M) \rangle} \right)$

control parameter: MPS bond dimension χ

We can characterize a variational optimum for given values of (D,χ)

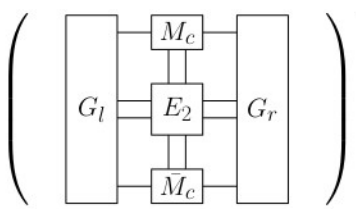
→ independent of contraction or optimization algorithm!

Variational optimization

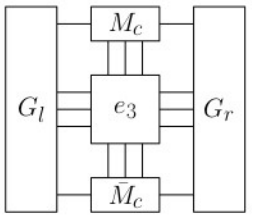
In practice, optimizing both variational principles can be done

→ boundary PEPS: gradient optimization (e.g., BLGS)

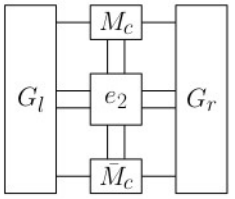
$$g = -\frac{2}{\lambda(A,\bar{A})}$$



$^{-1}$



$- \lambda(A,\bar{A})$



“Hellmann-Feynman theorem”: thanks to variational principle for the environment, the differentials of the environment tensors vanish

→ boundary MPS: vumps algorithm finds variational optimum

Overview

Introduction: PEPS for 2-D quantum systems and 3-D stat-mech

Variational optimization of PEPS fixed points

PEPS for critical systems: a scaling hypothesis

Outlook

Bram Vanhecke, Juraj Hasik, Frank Verstraete, LV
arXiv:2102.03143

PEPS for critical systems

Finite-size scaling in Monte-Carlo or exact diagonalization

Finite-entanglement scaling in MPS

for certain bond dimension, use effective correlation length as characteristic length scale

Nishino, Okunishi, Kikuchi, Phys. Lett. A 213, 69 (1996)

Tagliacozzo, de Oliveira, Iblisdir, Latorre, Phys. Rev. B 78, 024410 (2008)

Pollmann, Mukerjee, Turner, Moore, PRL 102, 25570 (2009)

For PEPS, situation is more complicated

algorithms give different results

- contraction: CTMRG, boundary-MPS, TRG and variations
- PEPS optimization: simple update, full update, variational optimization

two control parameters: two-step extrapolation?

high computational cost to get data points

PEPS for critical systems

Recently, a two-step procedure was proposed for extrapolating data

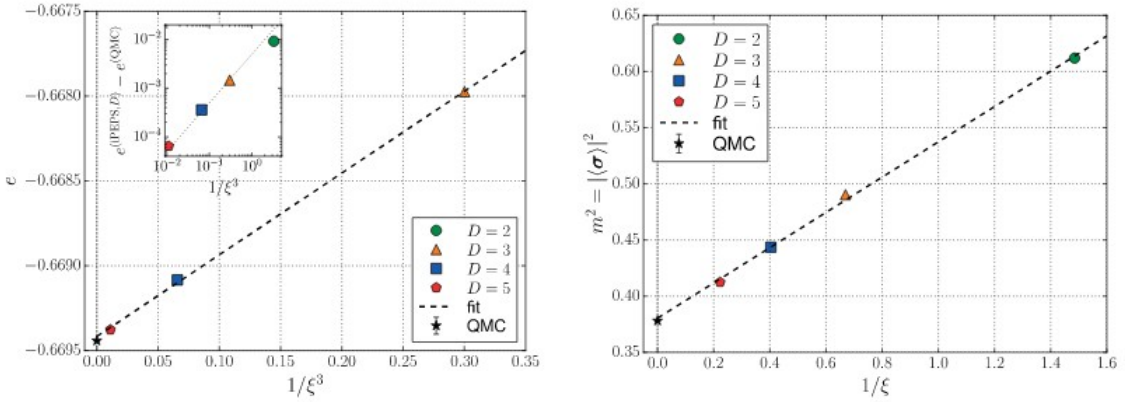
use variational optimization of PEPS tensors,
with χ large enough to get convergence

find PEPS correlation length by extrapolating
environment bond dimension

$$\xi_D = \lim_{\chi \to \infty} \xi_{\mathrm{boundary-MPS}}$$

Rader, Läuchli, PRX 8, 031030 (2018)

Corboz, Czarnik, Kapteijns, Tagliacozzo,
PRX 8, 6031031 (2018)



(taken from Rader & Läuchli)

→ needs very large χ to get a single data point

PEPS for critical systems

A scaling hypothesis for PEPS

→ place finite-D and finite-χ on an equal footing

PEPS for critical systems

A scaling hypothesis for PEPS

→ place finite-D and finite-χ on an equal footing

Procedure

characterize optimum by variational principles
for boundary PEPS *and* boundary MPS

extract correlation length from boundary MPS,
and formulate scaling hypothesis

$$O(D,\chi) = O(\xi_{\{D,\chi\}})$$

→ single effective length scale that models both finite-D and finite-χ effects

This approach is a lot more efficient

- one can get meaningful data for small χ
- a lot more data points for extrapolations

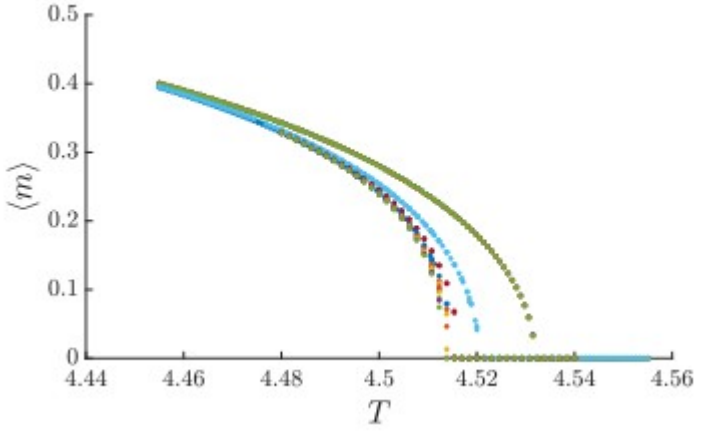
PEPS for critical systems

Application: classical 3-D Ising model

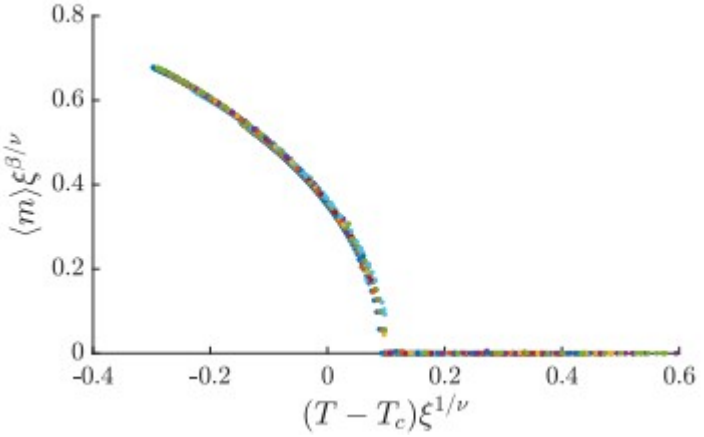
PEPS for critical systems

Application: classical 3-D Ising model

→ generate a lot of data points for different (D,χ)



→ apply scaling hypothesis to get data collapse



optimize data collapse
for critical temperature

$$T_c = 4.51170$$

current world record for TN,
dixit Nishino

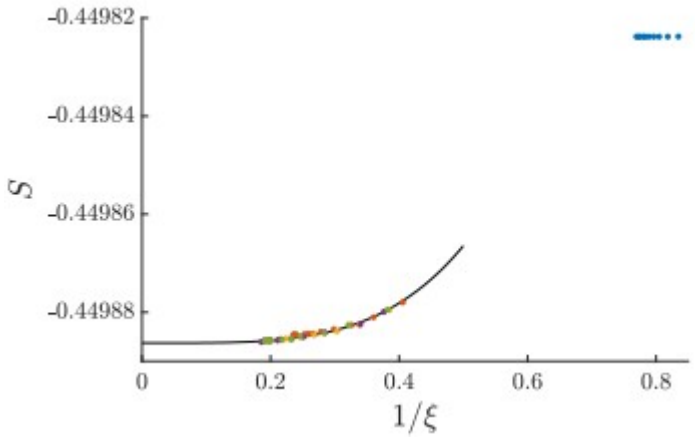
PEPS for critical systems

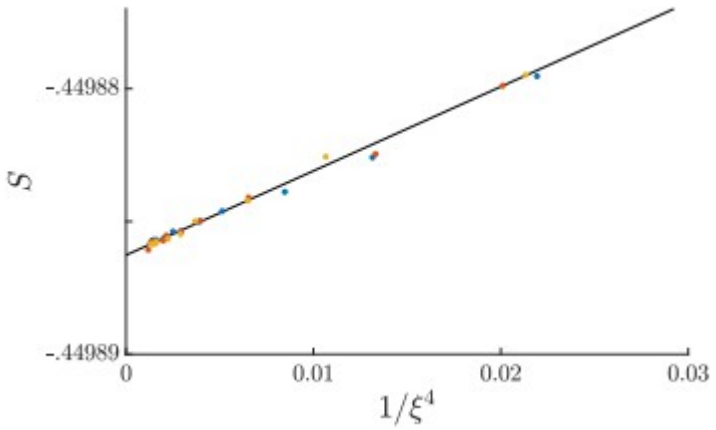
Application: 3-D dimer covering problem

PEPS for critical systems

Application: 3-D dimer covering problem

→ generate a lot of data points for different (D,χ)
and plot entropy vs inverse correlation length





We get unpredecented precision on the dimer entropy

$$S = 0.449886267(25)$$

compare to best MC result

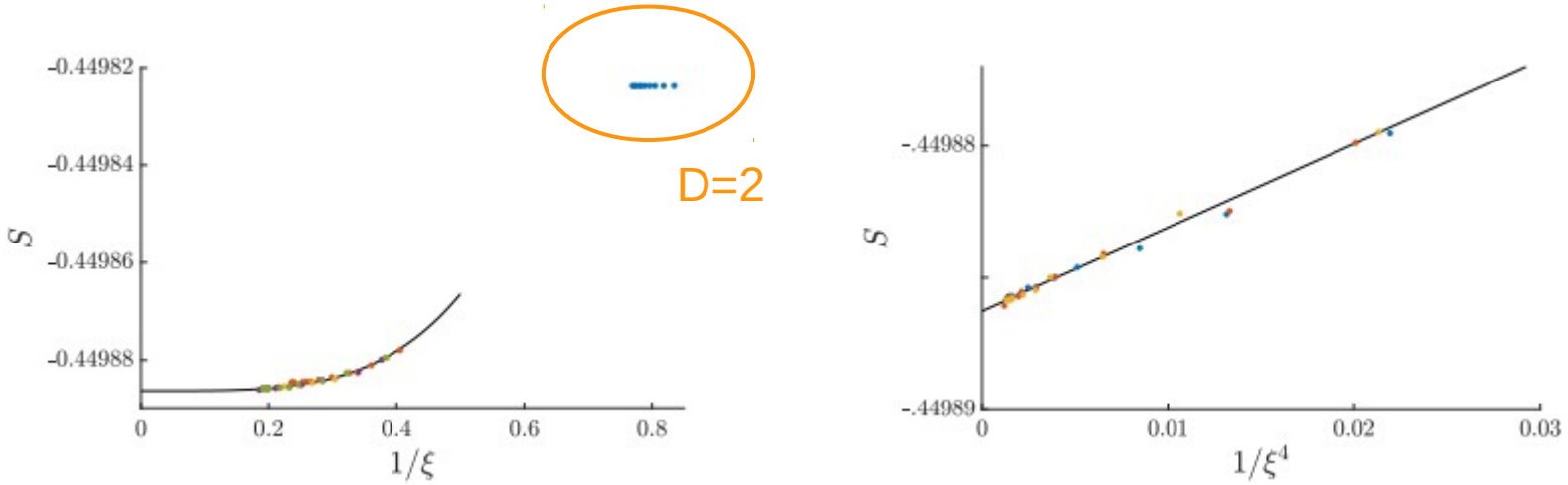
$$S = 0.4466(6)$$

Beichl, Sullivan, J. Comp. Phys. 149, 128 (1999)

PEPS for critical systems

Application: 3-D dimer covering problem

→ generate a lot of data points for different (D,χ)
and plot entropy vs inverse correlation length



We get unpredecented precision on the dimer entropy

$$S = 0.449886267(25)$$

compare to best MC result

$$S = 0.4466(6)$$

Beichl, Sullivan, J. Comp. Phys. 149, 128 (1999)

PEPS for critical systems

We can do the same procedure for 2-D quantum systems

PEPS for critical systems

We can do the same procedure for 2-D quantum systems

optimize PEPS tensor for variational energy,
evaluated with fixed environment bond dimension

use backwards differentiation for the cost function

$$e(A)_{\{D,\chi\}} = \frac{\langle \Psi(A) | \mathcal{H} | \Psi(A) \rangle_\chi}{\langle \Psi(A) | \Psi(A) \rangle_\chi}$$

Liao, Liu, Wang, Xiang, PRX 9, 031041 (2019)
Hasik, Poilblanc, Becca, SciPost Phys. 10, 012 (2021)

open-source software package for backwards differentiation of CTMRG contraction

J. Hasik and G. B. Mbeng, “peps-torch” (2020)

PEPS for critical systems

Application: 2-D quantum Heisenberg model

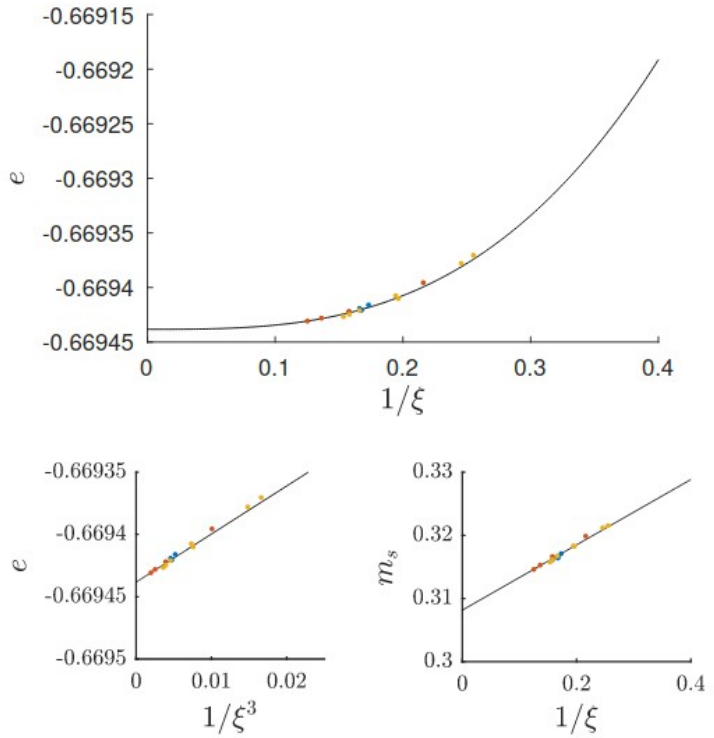


FIG. 3. Data for the 2-D Heisenberg model for $D = (6, 7, 8)$ and selected χ from 17 up to 200 for $D = 6, 7$ and 147 for $D = 8$. Top: energy vs. inverse correlation length of the environment MPS. Bottom-left: energy vs. the cube of the inverse correlation length. Bottom-right: magnetization vs that same inverse correlation length. Fits are performed on all the data and are shown in black.

optimize PEPS for different (D,χ)

energy/magnetisation vs inverse correlation length nicely collapses on a single curve

get extrapolated values

$$e = -0.6694401(10)$$

$$m_s = 0.30771(31)$$

compare to MC values

$$e = -0.669437(5)$$

$$m_s = 0.30743(1)$$

Sandvik, PRB 56, 11678 (1997)
Sandvik, Evertz, PRB 82, 024407 (2010)

Overview

Introduction: PEPS for 2-D quantum systems and 3-D stat-mech

Variational optimization of PEPS fixed points

PEPS for critical systems: a scaling hypothesis

Outlook

Bram Vanhecke, Juraj Hasik, Frank Verstraete, LV
arXiv:2102.03143

Outlook

Accurate PEPS simulations of (3+0)-D or (2+1)-D critical theories are possible

optimize at finite (D,χ) through variational principles

extract a single effective length scale from
optimized PEPS and environment

scaling hypothesis

Outlook

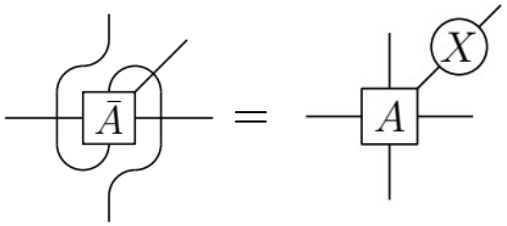
Accurate PEPS simulations of (3+0)-D critical theories are possible

optimize at finite (D,χ) through variational principles

extract a single effective length scale from optimized PEPS and environment

scaling hypothesis

Symmetry constraints on PEPS tensor



→ what ground states do not permit such a parametrization?

More exotic critical points

What about (3+1)-D systems?

→ 3 control parameters, 3-step hierarchy of variational principles, single effective length scale?

Thank you!